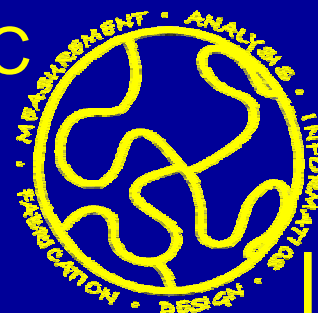


# Combinatorial Methodologies for Formulations: Industrial Needs for the 21<sup>st</sup> Century

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## Formulations:

- Definition of a Formulation
  - A multi-component fluid, often of mid-range viscosity (c.a. 100 centipoise, comparable to honey), with properties highly tailored to an industrial need, such as coatings, adhesives, lubrication, heat transfer, hydraulics, food additives, or hygiene-related consumer products.
- Critical Issues
  - The challenge is to develop high-throughput techniques to measure properties such as compatibility, stability, and properties related to the ultimate performance of the product.

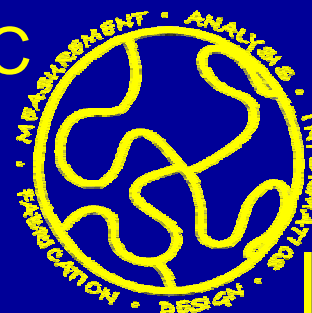
# Formulations Require Many Components

Individual components are mixed together to produce a formulation with the desired properties.



Formulations can include dozens of components!  
e.g. pigments, binders, rheology modifiers surfactants

**Challenge:** How do we determine the optimum amount of each component?



# Performance Properties to Optimize for Paints

## Application and Appearance

Properties

Colour

Hiding

Flow and Leveling

Level of Sheen Gloss

Spattering Tendency

Foaming Tendency

## Interior Paint Properties

Stain Resistance

Scrub Resistance

Lack of Yellowing

Resistance to Alkaline Clean

Burnish Resistance

Block Resistance

## Exterior Paint Properties

Colour retention

Mildew Resistance

Blister Resistance

Dirt Resistance

Resistance to Peeling

Alkali Resistance

**Any high-throughput test must take into account the product performance in its final application.**

Courtesy of  
Paint Quality Institute

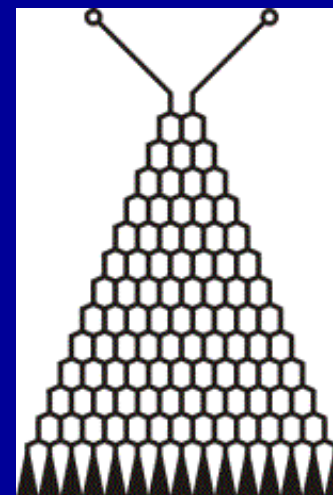
# Methods for Making Multicomponent Mixtures

Standard Model:  
Microwell array plate  
with robotically  
controlled dispenser



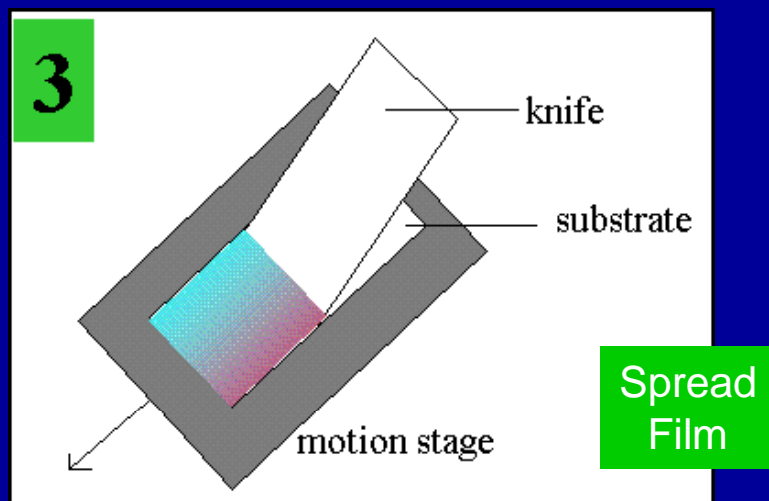
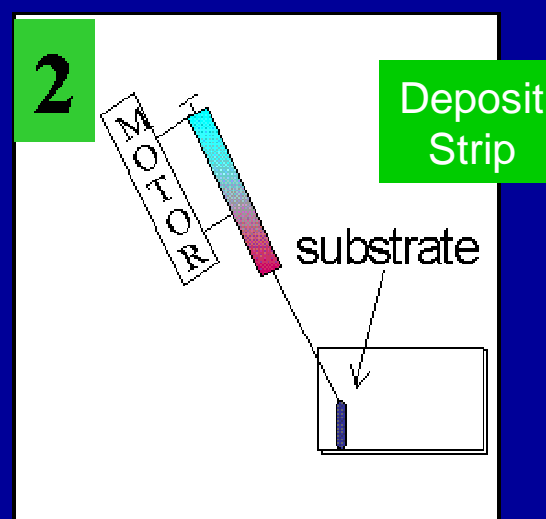
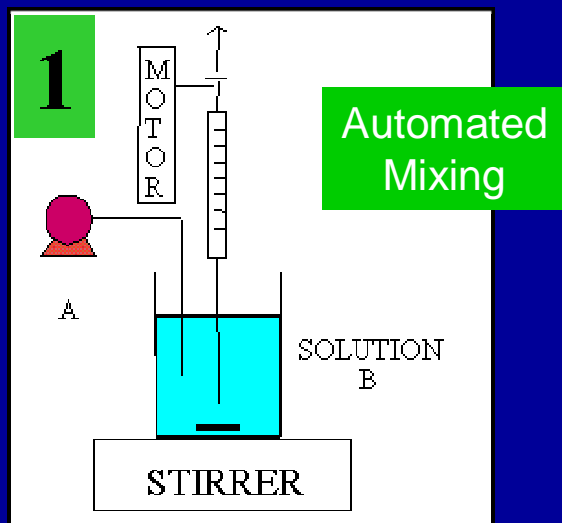
Wicks and Bach

Milli-fluidic mixer



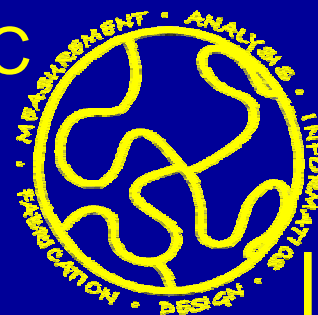
Scott Kennedy

# Compositional Gradient Apparatus

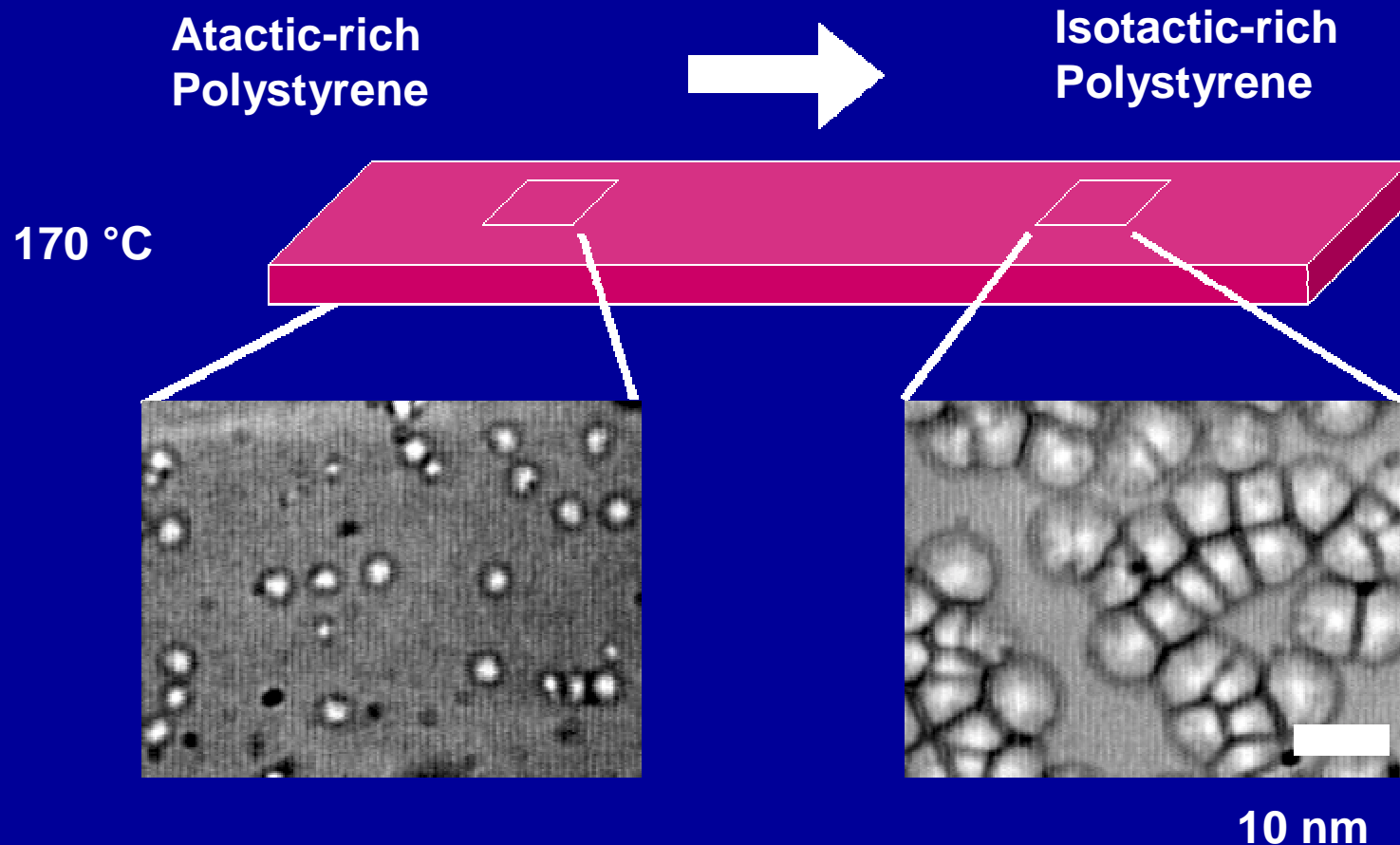


## CAVEATS/ LIMITED TO:

- Low viscosity solutions (10cp)
- Low solids content (1-4 %)
- Volatile solvents (e.g. toluene)
- Thin films (0.1-1 mm)

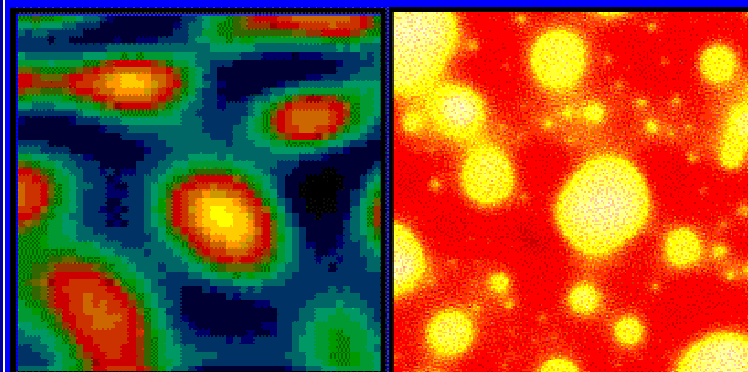
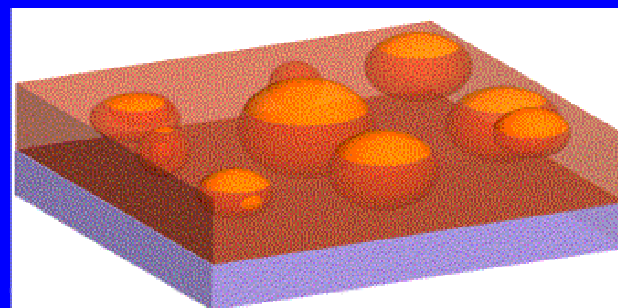
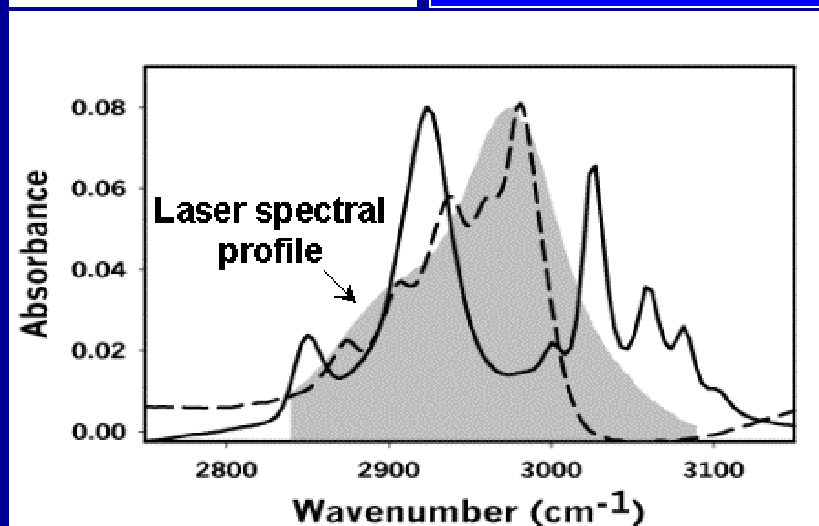
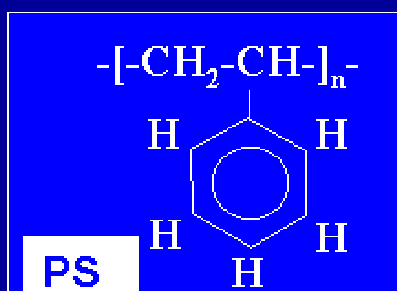
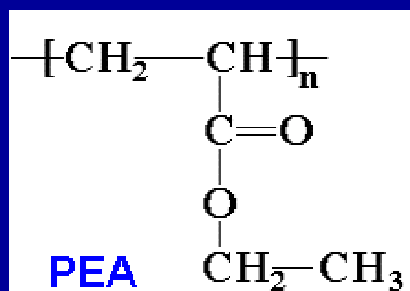


# Compositional Gradient Apparatus: Tacticity of Polystyrene on Crystallization Kinetics



Tacticity of polystyrene affects kinetics!

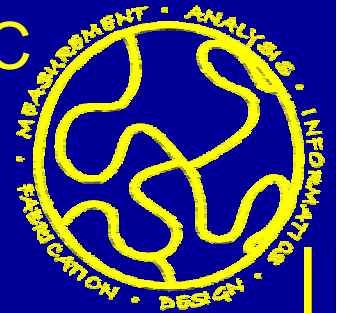
# IR Visualization of Coating



IR NSOM Transmission AFM Topography  
Different regions of sample: BOTH 8 x 8 μm

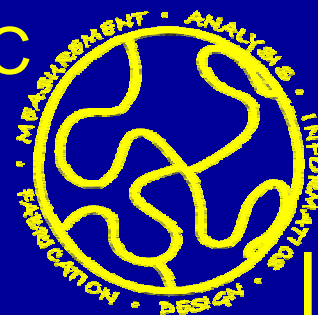
Courtesy: Steve Buntin

Group Leader, Surface and Interface Research Group  
Chemical Science and Technology Laboratory (CSTL) NIST



## Panel Discussion: What techniques should NIST be developing to assist industry?

- How do you determine which components to optimize (in quantity or quality) in a formulation?
- What strategies can/should we use to effectively employ combi techniques in complex formulations problems?



	Properties	Performance Properties	Test
Paints	Viscosity, Surface Tension	Modulus, Gloss, Impact Resistance	
Adhesives			
Microemulsions- Complex fluids			